

- times each atom type occurs for each ionizable group on each molecule of a series of molecules for which an experimentally determined pK_a is known;
- b) place each of the determined atom types noting the number of times each atom type occurs for each hierarchically determined connectivity tree in a row of a data table along with the experimentally determined pK_a of the molecule from which the tree was determined;
- c)[b.] using the partial least squares (PLS) statistical methodology, extract coefficients associated with each atom type represented at each hierarchical level;
- d)[c.] determine the hierarchical atom type connectivity tree noting the number of times each atom type occurs for the molecule of interest; and
- e)[d.] multiply the number of occurrences of each atom type in the molecule of interest by the PLS coefficient determined for that atom type and sum the resulting multiplications to obtain the predicted pK_a .
2. The method of claim 1 in which each atom type from the hierarchical atom connectivity tree in steps a and d[c] for each ionizable group on each molecule is placed into a separate bin in a bit string.

REMARKS

Applicants respond to the Examiner's remarks by reference to the Examiner's paragraph numbers in the Office Action.

Examiner's Paragraph 1:

The Examiner has kindly reminded applicants of the new time requirement for submission of revised drawings. Applicants have accordingly submitted revised drawings under separate letter addressed to the Official Draftsperson. As a courtesy to the Examiner, a